

Model Performance

Model

Data

Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -59.2 °C

Global applicability domain: Inside

Local applicability domain index: 5.11e-01

Confidence level: 5.93e-01

Nearest Neighbors from the Training Set

Image not found

Sarin

Measured: -57.0

Predicted: -59.2

Image not found

Pinacolyl

methylphosphonofluoridate

Measured: -42.0

Predicted: -48.2

Image not found

Diisopropyl fluorophosphate

Measured: -82.0

Predicted: -73.2

Image not found

Phosphonothioic acid, methyl-,
O,o-diethyl ester

Measured: -84.4

Predicted: -62.3

Image not found

Dimethyl hydrogen phosphite

Measured: -60.0

Predicted: -61.6